Nitrofurantoin 67-20-9 | DTXSID7020972

Model Performance

Model	Data	
Model	Dala	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 2.59

Global applicability domain: Inside

Local applicability domain index: 3.77e-01

Confidence level: 8.99e-01

Nearest Neighbors from the Training Set

Image not found

Dimethoate
Measured: 1.58
Predicted: 1.88

Image not found

Amitrole

Measured: 3.09 Predicted: 3.40 Image not found

Carbendazim Measured: 2.51 Predicted: 2.38

Image not found

Cyanoguanidine Measured: 3.09 Predicted: 2.93 Image not found

Bromacil Measured: 3.24 Predicted: 2.87